5/1/07 Lecture 9 outline

• Recall the eigenvalue equation for the allowed energies of a system,

$$H\psi_n \equiv \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi_n = E_n\psi_n.$$

The solutions of this equation (with appropriate boundary conditions) form a complete basis for possible wavefunctions. Any wavefunction (with appropriate BCs) can be written as a linear combination of them:

$$\psi(x) = \sum_n A_n\psi_n(x), \qquad \text{where} \qquad A_n = \int dx \psi_n^*(x)\psi(x).$$

The probability of measuring energy E_n is then $|A_n|^2$. (After the measurement of some E_n, the wavefunction collapses $\psi \to \psi_n$.)

We discussed this last week for the specific example of a particle in a box, but all the above statements are quite general.

• The time dependence of the wavefunction is given by the Schrodinger equation,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = H\psi.$$

Using the above form, we can immediately determine the solution of the Schrodinger equation. The wavefunction, as a function of time, is given by

$$\psi(x,t) = \sum_n A_n e^{-iE_nt/\hbar}\psi_n(x), \qquad \text{where} \qquad A_n = \int dx\ \psi_n^*(x)\psi(x,t=0).$$

Once we've expanded the initial wavefunction $\psi(x,t=0)$ in terms of the energy eigenstates (which is a useful thing to do in any case!), we can immediately write down the time dependence, as above! The S.E. is a partial differential equation, in x and t, and the solution above is the statement that we can use separation of variables, along with superposition (since the equation is linear).

• Even though the above t dependence looks so simple, it leads to very non-trivial t dependence when we compute different quantities, e.g. the position probability density $\rho(x,t) = |\psi(x,t)|^2$. This leads to nontrivial t dependence in general for measured quantities, and also for expectation values.

• Note that if the system is in an energy eigenstate, $\psi(x,t) = e^{-iE_nt/\hbar}\psi_n(x)$, then all expectation values like $\langle x^n\rangle$ and $\langle p^n\rangle$ are time independent. This is called a stationary state.

• Next topic, the step potential. Suppose

$$V(x) = V_0\theta(x), \qquad \theta(x) \equiv \begin{cases} 0 & x < 0 \\ 1 & x > 0. \end{cases}$$

We will solve the eigenvalue equation $H\psi = E\psi$. Suppose that there is an incoming flux from the left, with energy E. The wavefunction is then of the form

$$\psi_1(x) = e^{ik_1 x} + Re^{-ik_1 x},$$

where 1, is for the $x \le 0$ region. k_1 is given by $\hbar k_1 = \sqrt{2mE}$. In region 2, which is $x \ge 0$, we have

$$\psi_2(x) = Te^{ik_2 x}$$

where $\hbar k_2 = \sqrt{2m(E - V_0)}$. We chose the solution so that the wave only moves to the right in region 2, because we take the particle to be incoming from $x = -\infty$. The coefficient $|R|^2$ is the reflection probability coefficient and $|T|^2$ is the transmission probability coefficient (here I'm following the notation of Gas. - but note that many other books call his R a coefficient B and his T a coefficient C, and reserve the names R and T for what Gas is calling $|R|^2$ and $|T|^2$: $R_{others} = |R_{Gas}|^2$ and $T_{others} = |T_{Gas}|^2$.

We solve for R and T by noting that the wavefunction must be continuous. Moreover, for a smooth potential, the derivative of the wavefunction must also be continuous. So

$$1 + R = T \qquad ik_1(1 - T) = -k_2 T$$

gives

$$R = \frac{k_1 - k_2}{k_1 + k_2} \qquad T = \frac{2k_1}{k_1 + k_2}$$

The flux in region 1 is

$$J = \frac{\hbar}{2im}(\psi^*\psi' - \psi^{*\prime}\psi) = \frac{\hbar k_1}{m}(1 - |R|^2)$$

The flux in region 2 is

$$J = \frac{\hbar k_2}{m}|T|^2$$

Where

$$\frac{\hbar k_1}{m}|R|^2 = \frac{\hbar k_1}{m}\left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \qquad \frac{\hbar k_2}{m}|T|^2 = \frac{\hbar k_1}{m}\frac{4k_1 k_2}{(k_1 + k_2)^2}.$$

If $E < V_0$, then instead get $\psi_2(x) = Te^{-\kappa_2 x}$, where $\hbar\kappa_2 = \sqrt{2m(V_0 - E)}$. In that case, $|R|^2 = 1$. Find also $T = 2k_1/(k_1 + i\kappa_2)$.

• Comments on delta function potential, and how the ψ' matching is affected: integrate the S.E. across the delta function potential to get

$$-\frac{\hbar^2}{2m}\frac{d\psi}{dx}\Big|_{x-\epsilon}^{x+\epsilon} + \int_{x-\epsilon}^{x+\epsilon} V(x)\psi(x) = 0,$$

where the second term only contributes if $V(x)$ has a delta function. Then the above equation shows that ψ' has a specific discontinuity across that x.